

AN IMPROVED 2-D REACTIVE TRANSPORT MODEL OF THE FATE OF CO₂ INJECTED INTO A SALINE AQUIFER IN THE WABAMUN LAKE AREA (ALBERTA, CANADA)

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ABSTRACT

The Wabamun Area CO₂ Sequestration project (WASP) examined the feasibility of storing 20 million tons (Mt) of CO₂ per year over 50 years in a deep saline aquifer in central Alberta, Canada. In the WASP project, the Devonian Nisku saline aquifer was selected as the primary target for CO₂ injection. The reactive transport code TOUGHREACT was used to investigate CO₂-brine-rock interactions induced by the injection of supercritical CO₂ into the Nisku aquifer. Previously, 1-D and 2-D modeling studies of CO₂ storage in the Nisku Aquifer were performed. Here, we present an extended 2-D modeling study by considering five zones including the Nisku aquifer's three different flow units, the overlying shaly caprock (Calmar) and the underlying shale (Ireton) to obtain more accurate predictions of the fate of injected CO₂. The CO₂ was injected into the bottom 10 m of the Middle Nisku zone at a rate of 1 Mt/year for 50 years. The simulation results revealed that after 1 year, the buoyancy effect resulted in injected CO₂ rising from the Middle Nisku up to the Calmar shale and then expanding as a plume of supercritical CO₂ beneath this cap rock. The injected CO₂ plume spread out radially up to 3.5 km after 50 years of injection, and to 5 km after 1000 years post-injection. Due to dissolution of minerals (mainly dolomite), minor increases in porosity (0.2%) and permeability (2.5 md) of the Middle Nisku aquifer were observed within 3.5 km of the injection well during the 1000 years post-injection period.

The mineral-trapping capacity of injected CO₂ in the Nisku aquifer (mainly composed of carbonate rock) was found to be 0.18 Mt or <0.5% of the 50 Mt of injected supercritical CO₂. This indicates that the carbonate Nisku aquifer does not have a large mineral trapping capacity for CO₂ and that the majority of the

injected CO₂ is sequestered by hydrodynamic and solubility trapping mechanisms. The Calmar formation proved to be an excellent caprock for the CO₂ injected into the Nisku aquifer.

2-D simulation results also revealed that density driven flow resulted in CO₂ migrating down from the storage Nisku aquifer to the underlying Ireton formation. The Ireton shale is rich in aluminosilicates such as k-feldspar, albite and chlorite. After 1000 years, it was observed that this shale has a large capacity for mineral trapping of injected CO₂ of up to 20 kg of injected CO₂ per m³ rock in immobile forms such as ankerite and dolomite.

The results from this 2-D modeling study suggest that the Nisku aquifer is a suitable formation for CO₂ storage in the Western Sedimentary Basin in Canada (WSBC) in terms of geochemistry, injectivity, storage capacity and cap rock integrity. Also, the underlying shale has the potential to sequester CO₂ in mineral (carbonate) form.

INTRODUCTION

Carbon Capture and Storage (CCS) has been considered for a long time as an option to mitigate increasing human-induced greenhouse gas emission to the atmosphere and meet future emission goals. Before CCS becomes fully operational at commercial scale, its long-term impacts and risks associated with human and environmental safety must be assessed. Numerical modeling of CO₂ storage plays an important role in making predictions of short- and long-term behavior of injected CO₂ in geological formations and to help to give insights into its long-term fate via different physical and chemical trapping mechanisms over time.

The WSBC has been the subject of many studies evaluating the potential for CO₂ storage and investigating its hydrogeology, geochemistry, CO₂ storage capacity and CO₂ trapping mechanisms (Bachu et al., 1994, Gunter et al., 1993, 1996). The Wabamun Area CO₂ Sequestration project (WASP) examined the feasibility of storing 20 Mton-CO₂/year over 50 years in central Alberta, Canada (Lavoie and Keith, 2010). In the WASP project, the Devonian Nisku aquifer was selected as the primary target for CO₂ sequestration. Previously, a 1-D modeling study of the fate of injected CO₂ in the Nisku Aquifer was performed to assess the effect of presence of H₂S on CO₂ storage. It was found that H₂S appeared to have little effect on the modeled CO₂-brine-rock reactions in the Nisku aquifer (Shevalier et al., 2011). For the present study, the objective was to develop a 2-D model with three different flow units in the Nisku formation that were observed in petrophysical analyses. The goal was to increase the accuracy of predicting the behavior of the injected CO₂ in the formation and to predict hydrodynamic, solubility, and mineral trapping mechanisms over the simulation time.

THE STUDY AREA

The Devonian Nisku formation in Central Alberta was identified as a potential aquifer for CO₂ injection in the WASP project. It is located in the southwest of Edmonton, Alberta with a total areal extent of approximately 5034 km² (Figure 1). The Nisku aquifer was selected because of its depth, good reservoir qualities and lack of oil and gas activities in the area of interest. It was also well suited regarding the delicate balance between the availability of data (number of penetrating wells) and the risk of leakage through wells. No fault through which the injected CO₂ could release back to surface was detected in the seismic survey and interpretations. A number of large stationary CO₂ sources are located in central Alberta with total CO₂ emission of 30Mt/year including four coal-fired power generation plants with more than 4000 MW/year total generating capacity in the Wabamun Lake area. The estimated CO₂ emission from these four power plants is 3-6 Mt/year.

NUMERICAL TOOL

All of the simulations were performed using TOUGHREACT v. 1.2 (Xu and Pruess, 2001). The code was based on the existing multi-phase fluid and heat flow code, TOUGH2 v. 2 (Pruess, 1991) and the geochemical reactive transport code was added. The integral finite difference method for space discretization (Narasimham and Witherspoon, 1976) is the basis for the numerical method for simulation of fluid flow. The coupling between the geochemical reactions and the fluid transport is a sequential iterative approach (Yeh and Tripathi, 1991). The fluid property module ECO2N was used in the modeling.

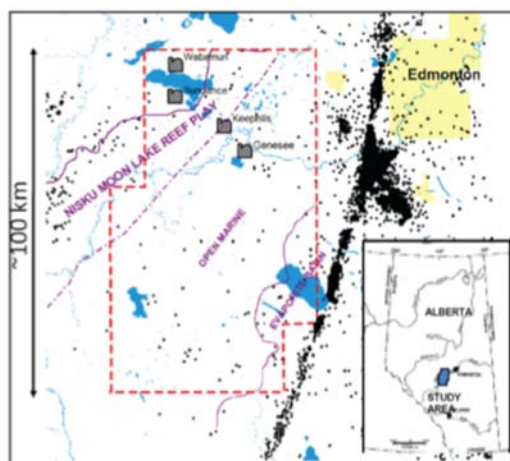


Figure 1. The study area (dashed line) in central Alberta (Canada) with the location of four large power plants. Black circles show well that penetrate the Nisku Formation (Shevalier et al., 2011).

MODEL SETUP

A 2-D radially symmetric model was created in TOUGHREACT/Petrasim for a CO₂ injection into the Devonian Nisku saline aquifer (Figure 2). Three different zones of the Nisku aquifer (the Upper, Middle and Lower Nisku) were introduced into the 2-D model. These different flow regimes in the Nisku formation were identified by petrophysical analyses during the WASP project. The overlying (Calmar shale) cap rock and underlying (Ireton shale) formation were also considered in the model. The model is 90 m thick and 20 km wide in radial distance. The first upper 10 m represents the Calmar cap rock, the next 15 m is the Upper Nisku, and the

following 20 m is the Middle Nisku. The Lower Nisku is 35 m thick, and the remaining 10 m represents the Ireton shale. CO₂ was injected into the bottom 10 m of the Middle Nisku (between 35–45 m in the model), which is the most permeable and porous zone in the Nisku formation.

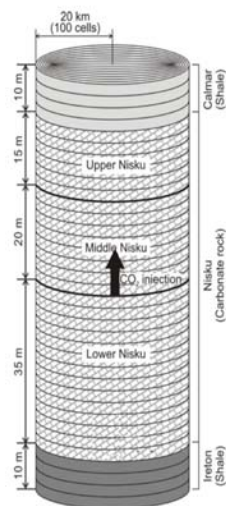


Figure 2. 2D-Model representation formation.

INITIAL GEOCHEMICAL CONDITIONS

Hydrogeological parameters of the Calmar, the Upper, Middle and Lower Nisku and Ireton formations defined in the model are given in Table 1. The Middle Nisku is the most porous and permeable zone, with a porosity of 21.9% and a permeability of 91 md. The overlying Calmar shale is impermeable with a permeability value of 2.9×10^{-6} md, suggesting that it is an excellent cap rock. The van Genuchten (1980) model was used to calculate the capillary pressure and relative permeability curves for each zone in the model.

Table 2 summarizes the measured water composition of brine obtained from a water-producing well located in the Nisku formation (Shevalier and Mayer, 2009). The Nisku brine is “sour,” containing a considerable amount of H₂S gas. Within the scope of this modeling work, the content of H₂S was not considered. Shevalier et al. (2011) previously revealed that H₂S appears to have little impact on the fate of the injected CO₂ in the Nisku aquifer.

The initial mineral compositions of a representative sample from the Calmar, Nisku, and Ireton formations used in the modeling are shown in Table 3 (Nightingale et al., 2009). The Calmar is composed of mainly quartz (48.16%), illite (29.28%), k-feldspar (17.31%) and minor amounts of low-albite, pyrite and calcite. The Nisku is a carbonate formation, consisting of mostly dolomite (over 80% in all its three zones). The Ireton is composed of illite (around 40%), calcite (27.36%), quartz (9.82%), k-feldspar (8.42%) and minor amounts of dolomite, chlorite, low-albite and pyrite.

The interaction between the reactive or more acidic fluids caused by CO₂ injection and storage rock minerals is a complex interplay between thermodynamic stabilities, reaction kinetics, and fluid flow. Table 4 provides the parameters for dissolution and precipitation kinetics for the minerals used in the models (Palandri and Kharaka, 2004). Calcite was used as an equilibrium mineral in the simulations: its kinetics are comparably fast. Mineral disequilibria induced by CO₂ injection results in dissolution of primary minerals and precipitation of new, secondary minerals stable at elevated CO₂ pressure. Table 2 shows the secondary minerals considered in the 2-D model.

Table 1. Hydrogeological parameters for the Calmar, Nisku and Ireton formations

	Calmar	Upper Nisku	Middle Nisku	Lower Nisku	Ireton
Porosity(%)	3.9	2.9	20.9	5.1	5.0
Permeability(m2)	2.9×10^{-21}	2.03×10^{-15}	9.1×10^{-14}	1.93×10^{-14}	1.0×10^{-16}
Temperature	70				
Pore Compressibility(Pa-1)	1.07×10^{-7}				
Diffusivity(m2/s)	1.0×10^{-9}				
Torosity	0.3				

Table 2. Initial chemical species concentrations of saline aquifer water used in the ToughReact simulations.

Species	Concentration (mol/kg)	Species	Concentration (mol/kg)
pH	6.1	SiO _{2(aq)}	4.56×10^{-4}
Ca ²⁺	0.41	HCO ₃ ⁻	2.01×10^{-2}
Mg ²⁺	9.33×10^{-2}	SO ₄ ²⁻	5.21×10^{-3}
Na ⁺	2.56	Cl ⁻	3.44
K ⁺	0.1	AlO ₂ ⁻	1.36×10^{-7}
Sr ²⁺	1.08×10^{-2}	O _{2(aq)}	4.88×10^{-70}
Fe ²⁺	9.35×10^{-6}		

Table 3. Mineralogical compositions of the Calmar, Nisku, and Ireton formations

<i>Primary Minerals</i>	Calmar (%)	Upper Nisku(%)	Middle Nisku(%)	Lower Nisku(%)	Ireton(%)
Dolomite		89.2	81.2	91.6	5.7
Calcite	0.5	6.2	15.5	4.7	27.4
Illite	29.3	2.0	1.9	0.5	40.0
K-feldspar	17.3	0.2	0.9	0.4	8.4
Quartz	48.2	2.0			9.8
Low-Albite	3.7		0.6		3.7
Pyrite	1.1				0.7
Chlorite					4.4
<i>Secondary Minerals</i>					
Kaolinite	Ankerite	Ca-smectite	Anhydrite	Aragonite	
Na-smectite	Magnesite	Dawsonite	Siderite		

Table 4. Parameters for calculating kinetic rate constants of minerals considered in the simulations (Palandri & Kharaka, 2004)

Mineral	S. Area (cm ² /g)	Parameters for kinetic rate law							
		Neutral mechanism		Acid mechanism			Base mechanism		
		k ₂₅	E _a	k ₂₅	E _a	n(H ⁺)	k ₂₅	E _a	n(H ⁺)
		(mol/m ² /s)	(kJ/mol)	(mol/m ² /s)	(kJ/mol)		(mol/m ² /s)	(kJ/mol)	
Dolomite	9.8	2.951×10 ⁻⁸	52.2	6.457×10 ⁻⁴	36.1	0.5			
Illite	151.6	1.660×10 ⁻¹³	35	1.047×10 ⁻¹¹	23.6	0.34	3.02×10 ⁻¹⁷	58.9	-0.4
K-feldspar	9.8	3.891×10 ⁻¹³	38	8.710×10 ⁻¹¹	51.7	0.5	6.310×10 ⁻²²	94.1	-0.82
Low-albite	9.8	2.754×10 ⁻¹³	69.8	6.918×10 ⁻¹¹	65	0.457	2.512×10 ⁻¹⁶	71	-0.57
Kaolinite	108.7	6.918×10 ⁻¹⁴	22.2	4.898×10 ⁻¹²	65.9	0.777	8.913×10 ⁻¹⁸	17.9	-0.47
Na-smectite	108.7	1.660×10 ⁻¹³	35	1.047×10 ⁻¹¹	23.6	0.34	3.02×10 ⁻¹⁷	58.9	-0.4
Ca-smectite	108.7	1.660×10 ⁻¹³	35	1.047×10 ⁻¹¹	23.6	0.34	3.02×10 ⁻¹⁷	58.9	-0.4
Dawsonite	9.8	1.260×10 ⁻⁹	62.76	6.457×10 ⁻⁴	36.1	0.5			
Aragonite	9.8	4.571×10 ⁻¹⁰	23.5	4.169×10 ⁻⁷	14.4	1			
Siderite	9.8	1.260×10 ⁻⁹	62.76	6.457×10 ⁻⁴	36.1	0.5			
Ankerite	9.8	1.260×10 ⁻⁹	62.76	6.457×10 ⁻⁴	36.1	0.5			
Magnesite	9.8	4.571×10 ⁻¹⁰	23.5	4.169×10 ⁻⁷	14.4	1			
Quartz	9.8	1.023×10 ⁻¹⁴	87.7						
Chlorite	9.8	3.02×10 ⁻¹³	88	7.762×10 ⁻¹²	88				
Pyrite	12.87	2.818×10 ⁻⁵	56.9 n(O _{2(aq)})=0.5	3.202×10 ⁻⁸	56.9	n(H ⁺)=-0.5 n(Fe ³⁺)=-0.5			

THE CO₂ INJECTION AND POST INJECTION SIMULATIONS

Simulations were performed using the reactive transport code TOUGHREACT. Injection of supercritical CO₂ was simulated into the bottom 10 m of the Middle Nisku formation at a rate of 1 Mton/year (31.69 kg/sec) for 50 years. Following the 50-year injection simulation, a simulation of 1000 years of post-injection was

conducted to understand the long-term behavior of the injected CO₂ in the reservoir.

RESULTS AND DISCUSSION

The simulation results are presented in 2-D graphical plots as a function of depth and radial distance at discrete time intervals of 1 and 50 years for the CO₂ injection and 100 and 1000 years for the post injection.

CO₂ Injection Phase

Since supercritical CO₂ is less dense than the formation brine, the injected CO₂ migrated up from the injection point toward the Calmar cap rock. Due to the rapid upward migration of the supercritical CO₂, a plume started to form beneath the cap rock 1 year after commencement of CO₂ injection, spreading radially up to 3.5 km after 50 years of injection (Figure 3). During the 1st year of injection, the CO₂ plume remained within the Nisku formation; however, at the end of the 50-year injection period, it was observed that some supercritical CO₂ entered the underlying Ireton shale, which has a considerably permeability. In contrast, the CO₂ did not diffuse into the Calmar cap rock over the simulation time, suggesting that the Calmar is an excellent cap rock. A dehydrated region with a radial distance of 100 m was observed forming due to complete brine displacement by the supercritical CO₂ injected at a high rate of 31.69 kg/sec. In Figure 3, CO₂ saturations of up to 1.0 were observed in this region. Figure 4 shows that the pH of brines in the Nisku aquifer decreased to a value of ~5.0 in areas affected by the injection as the supercritical CO₂ dissolved in the brine. The acidic brine subsequently dissolved dolomite, which is the main mineral in the Middle Nisku (Figure 5), resulting in increased Mg²⁺ ion concentrations in the reservoir brine (Figure 6). No increase in Ca²⁺ concentration in the brine was observed, which was explained by the precipitation of calcite that took up the Ca²⁺ released by dolomite dissolution (not plotted).

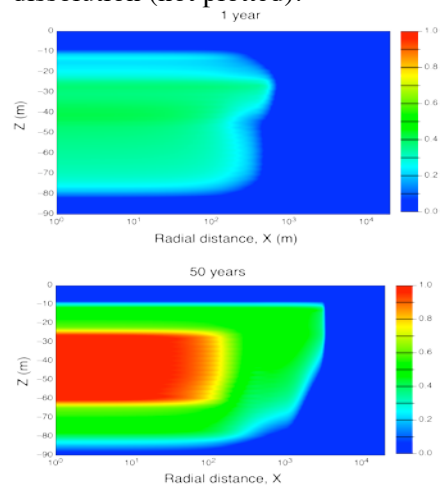


Figure 3. Spatial distribution of CO₂ plume after 1 and 50 years of injection

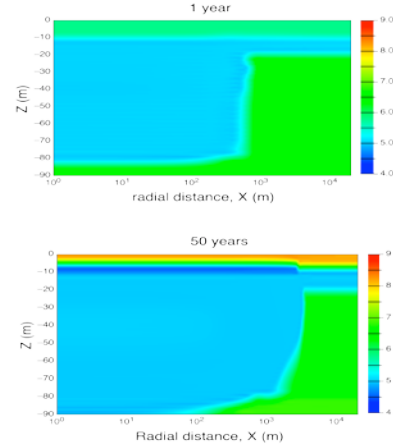


Figure 4. Spatial distribution of pH after 1 and 50 years of injection

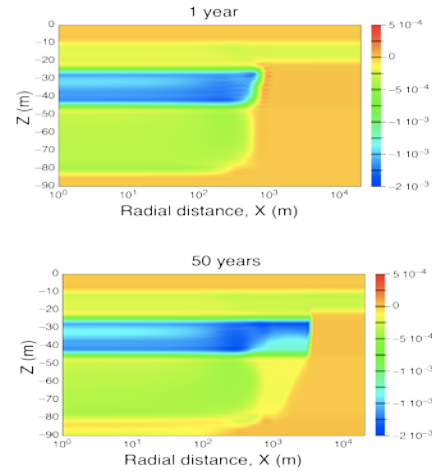


Figure 5. Change in volume fraction of dolomite after 1 and 50 years of injection

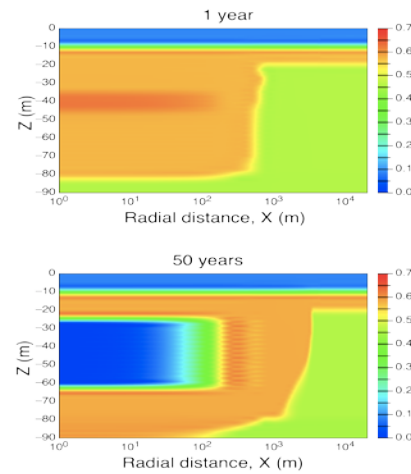


Figure 6. Mg²⁺ ion concentration after 1 and 50 years of injection

Post Injection Phase

Following the CO₂ injection simulation, a post-injection of 1000 years was simulated to evaluate the long-term fate of CO₂ injected into the Nisku aquifer. Also, the effect of geochemical reactions on formation porosity and permeability due to the CO₂ injection was investigated. The simulation result showed that after 1000 years of post injection, the injected supercritical CO₂ did not completely dissolve in the brine, with CO₂ saturations of up to 0.60 in parts of the Nisku aquifer. The plume was extended radially up to 5 km by capillary force, although the injection ceased after 50 years. It was observed that the CO₂ that migrated down into the Ireton shale during the injection was completely dissolved in its brine (Figure 7).

At the base of the Lower Nisku, it was observed that CO₂ was residually trapped after 1000 years. Dolomite dissolution was still ongoing in the Middle Nisku (Figure 8). Dissolution of calcite and chlorite in the Ireton shale (not shown) liberated divalent ions such as Ca²⁺, Mg²⁺ and Fe²⁺. Subsequently, dolomite (Figure 8, the bottom 10 m) and ankerite (Figure 9) were forming in the shale. Due to precipitation of these secondary minerals, the CO₂ mineral-trapping capacity was calculated as ~20 kg of CO₂/m³ rock in the Ireton formation (Figure 10). Dolomite dissolution in the Middle Nisku caused minor increases in porosity (by 0.2%) and permeability (by 2.5 md) (Figure 11).

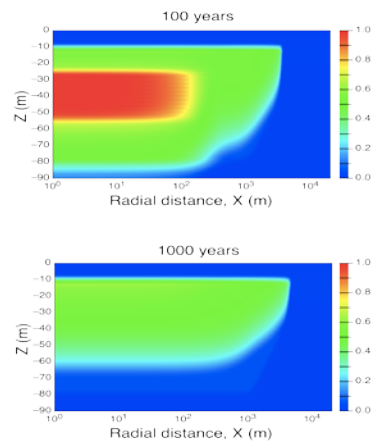


Figure 7. Spatial distribution of CO₂ plume after 100 and 1000 years of post injection

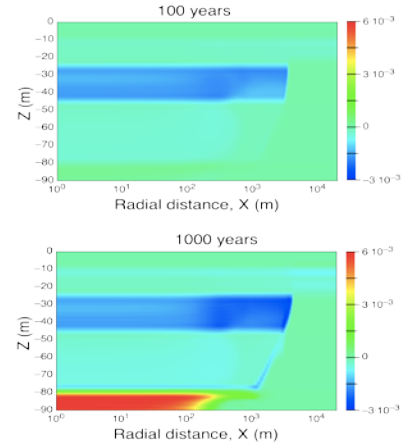


Figure 8. Change in volume fraction of dolomite after 100 and 1000 years of post injection

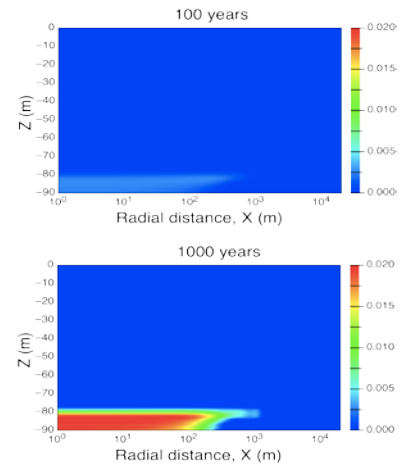


Figure 9. Change in volume fraction of ankerite after 100 and 1000 years of post injection

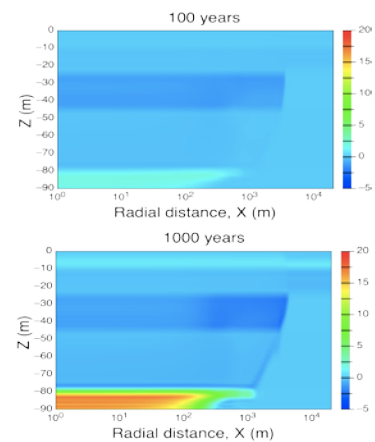


Figure 10. CO₂ mineral trapping after 100 and 1000 years of post injection

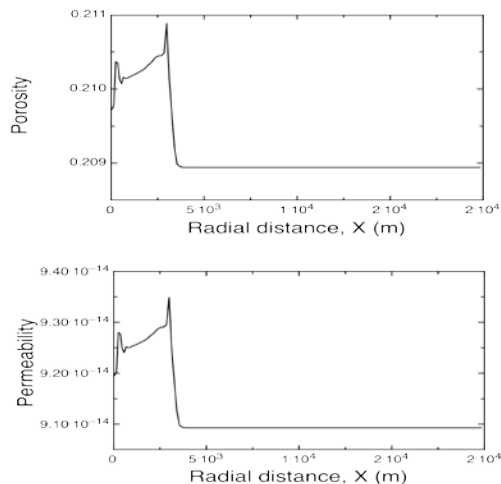


Figure 11. Change in the porosity and permeability of the Nisku aquifer

CONCLUSION

Storage of CO₂ in the Devonian Nisku aquifer in the WSBC was simulated using the multiphase, multicomponent and nonisothermal reactive transport TOUGHREACT code. The 2-D radially symmetric model developed in this work included the three different zones of the Nisku storage aquifer, along with its overlying cap rock and underlying shale. CO₂ injection caused acidification of the reservoir brine and some dissolution of dolomite in the Middle Nisku zone. This resulted in minor increases in the porosity and permeability of the Middle Nisku, although calcite was precipitating in this area. Since the Nisku formation is composed of carbonates, CO₂ mineral trapping was not a major sequestration process over the simulation period. Only 0.18 M tons of CO₂ were trapped as calcite mineral in the Nisku aquifer after 1000 years. The majority of injected CO₂ was trapped in free phase and as dissolved inorganic carbon in the brine. However, some injected CO₂ had also entered the underlying Ireton shale and dissolved in the brine, causing dissolution of calcite and chlorite. These mineral dissolution reactions liberated divalent cations into the brine, and dolomite and ankerite precipitated. The CO₂ mineral trapping capacity of the Ireton formation was calculated as up to 20 kg of CO₂ per m³ of rock. The impermeable Calmar shale proved to be an excellent cap rock for the CO₂ injected into the Nisku aquifer. This simulation study helped to make better predictions on the interactions of the reactive fluids and minerals of

the caprock, the storage reservoir, and the underlying formation induced by CO₂ injection.

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